

Chemical Space

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July 13, 2559 BE

```
library(caret)
library(reshape2)

df <- read.csv("data.csv")
names <- c("Activity", "SubFPC171", "SubFPC5", "SubFPC1", "SubFPC298", "SubFPC2", "SubFPC16", "SubFPC17",
           "SubFPC100")
df <- df[, names]
data_melt <- melt(df)
ggplot(aes(y = value, x = variable, fill = Activity), data = data_melt) + geom_boxplot() +
  ylab("Substructure Count") + theme(
    legend.position = "none",
    axis.text.y = element_text(size = 20, colour = "black"),
    axis.text.x = element_text(size = 20, colour = "black"),
    plot.margin = unit(c(1,1, 1, 1),"cm"),
    panel.border = element_rect(linetype = "solid", colour = "black", fill = NA, size = 1),
    axis.title = element_text(size = 25, face = "bold", colour = "black")
  )
```

